

Comprehensive biological evaluation (DNA-binding, cleavage, and antimicrobial activity) of β -diketimine Schiff base ligands and their Cu(II) and Zn(II) complexes

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Abstract

This article focuses on the combination of Cu(II) and Zn(II) ions with sulfur derivatives having Knoevenagel condensate β -diketimines and their pharmacological evaluation. Characterization of these complexes was done by usual spectroscopic and analytical techniques. The observed data demonstrate that the complexes have 1:1 (metal:Schiff base derivative) stoichiometry, $[MLCl_2]$ (where M = Cu(II) and Zn(II); L = Schiff base derivatives) and adopt square-planar geometry. From the results of *in vitro* DNA-tailoring bioassay studies (UV-vis, cyclic voltammetry, viscosity, and gel electrophoresis techniques) minor-groove-binding mode is exhibited between the synthesized compounds and the target CT-DNA. Moreover, they effectively cleave the supercoiled pBR322 DNA. Pharmacokinetic behavior is studied by SWISS ADMET online software. The optimized geometry and the quantum mechanical examinations of the synthesized compounds are carried out in Gaussian 09 W software by using B3LYP method, which implies that the nitro compounds have higher biological profile than other compounds. The *in vitro* antimicrobial screening impact has been performed against different microorganisms by well dispersion method. It has been found that the antimicrobial efficacy of the Schiff base is expanded on complexation with metal ions. Molecular docking study has been carried out on the cyclooxygenase (6-COX) enzyme for all the synthesized compounds.

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